AD-A154 126 THEORETICAL INVESTIGATION OF MATERIAL CHARACTERISTICS OF SEMICONDUCTOR SUPERLATTICES(U) MARYLAND UNIV COLLEGE PARK DEPT OF PHYSICS AND ASTRONOMY S D SARMA APR 85 1/1

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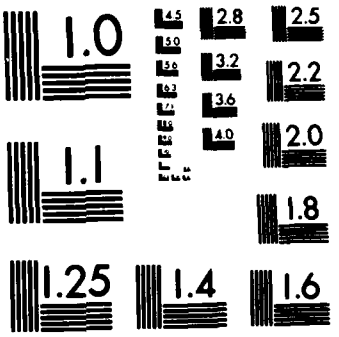

Annual Technical Report on Contract No. N00014-84-K-0586

"Theoretical Investigation of Material Characteristics of Semiconductor Superlattices"

Submitted by:

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April 1985

I. Progress during Period - Year 1

In the last six months that we had this contract we have been able to initiate all phases of the proposed work, making substantial progress on a number of research areas covering the many different aspects of the contract. In particular, we have written nine papers (six of which have already been published or accepted for publication) and have submitted seven abstracts to conferences. We have done enough work for several more publications and these papers are in preparation. We also plan to submit three papers to the upcoming 2nd International Conference on Metastable and Modulated Semiconductor Structures (September 1985 in Japan) and three papers to the upcoming 6th International Conference on Electronic Properties of Two Dimensional Systems (September 1985). Brief outlines of our progress in various areas are given in the following:

(1) Molecular Dynamics (MD) study of interface kinetics in semiconductor superlattices

We have been extremely fortunate in convincing the University of Maryland Computer Center to provide us for free with almost $100,000 worth of computing time at the Mainframe Univac 1182 system. We have already implemented a large MD program which is running. We have interesting results for atomic self-diffusion at interfaces as a function of layer number, temperature, atomic density, and interface roughness. We find an interesting correlation between the diffusion coefficient and the number of layers involved. This work is proceeding at a tremendous pace (about 100 hours worth of mainframe computing per week!!) and we can really use a mini-computer (e.g. VAX 780) of our own. We expect a preprint to be ready on this subject within the next one month. We are presenting a paper on the diffusion work at the APS March meeting at Baltimore. The PI has also been invited to give an invited talk on the subject at the

Greater Washington Area Statistical Physics Symposium. We plan to submit a paper to the Japan Conference covering this work.

(2) Epitaxial growth

This phase of the work has been slightly delayed by the late arrival of our Research Associate Dr. Akiko Kobayashi. Currently, we are looking at the fundamental aspect of epitaxy energetics, and, how strain, dislocations, misfits and vibrations affect the epitaxial energetics by studying a model interface within generalized rigid-atom picture (generalized Van der Merwe model). We expect to be able to get a good qualitative feel for defect energetics in epitaxial growth on the basis of this work. We will submit one paper to the Japan Conference on this work.

(3) Monte-Carlo (MC) simulation of superlattice growth

After reviewing the literature on this subject we have concluded that most of the work on this subject is either incorrect, or too simple-minded to be of any use. We are developing a MC algorithm with a realistic model where our MD results will be used as input parameters. This is another area where we can really use our own minicomputer. We will submit one paper to the Japan Conference on this subject.

(4) Electronic properties of superlattices

We have made significant progress in studying the electronic properties of superlattices by studying screening effects on hot-electron properties and by doing a detailed analysis of the electron-phonon interaction in the GaAs based system. This work has attracted widespread attention. We have also studied optical properties of (recently fabricated) Quantum well wires and other narrow channel systems which have projected applications as lateral 2D superlattices. In another paper we have investigated the role of impurity in the Fractional Quantum Hall effect phenomenon.

(5) Adsorption interaction

We have theoretically investigated the atomic adsorption on surfaces and find that the simple Van der Waals interaction which is universally used in physisorption work is inapplicable. We have obtained the correct adsorption potential.

(6) Self-trapping due to lattice interaction

We have carried out a detailed adiabatic analysis as well as a numerical quantum path-integral calculation of this very important problem. Our results establish, for the first time, qualitative criteria controlling the self-trapping problem.

Publications under ONR Contract (PI: S. Das Sarma)

1. Band non-Parabolicity Effects on Weak-Coupling Polarons in Compound Semiconductors (S. Das Sarma and B.A. Mason), Phys. Rev. (Rapid Communication) B 31, 1177 (1985).
2. Optical Phonon Interaction Effects in Two-Dimensional Semiconductor Microstructures (S. Das Sarma and B.A. Mason), Annals of Physics (in press).
3. Higher Order Corrections to Physisorption Interaction between an Adsorbed Atom and a Metal Surface (S. Das Sarma and S.M. Paik), Chem. Phys. Lett. (in press).
4. On the Self-Trapping of an Electron Due to Lattice Interaction (S. Das Sarma), Solid State Commun. (in press).
5. Polaron Quasi-particle Spectrum in Two Dimensions (B.A. Mason and S. Das Sarma), Phys. Rev. B (in press).
6. Screening of Polar interaction in Quasi-Two Dimensional Semiconductor Microstructures (S. Das Sarma and B.A Mason), Phys. Rev. B (in press).
7. Screening and Elementary Excitations in Narrow Channel Semiconductor Microstructures (S. Das Sarma and W.Y. Lai), submitted to Phys. Rev. Lett.
8. Effect of a Charged Impurity on the Fractional Quantum Hall Effect: An Exact Numerical Study (F.C. Zhang, V. Vulovic, Y. Guo and S. Das Sarma), submitted to Phys. Rev. Lett.
9. On the Saturation of the Van der Waals Potential near a Solid Surface (S. Das Sarma and S.M. Paik), submitted to Phys. Rev. B (Rapid Communications).

Papers to be Presented at Conferences

1. Atomic Self-Diffusion at Interfaces (E. Khor and S. Das Sarma), APS March Meeting at Baltimore (1985).
2. Screening and Elementary Excitations in Narrow Channel Semiconductor Microstructueres (W.Y. Lai and S. Das Sarma), APS March Meeting at Baltimore (1985).
3. Screening of Polar Interaction in Semiconductor Microstructures (S. Das Sarma and B.A. Mason), APS March Meeting at Baltimore (1985).
4. Path Integral Study of the Generalized Polaron Problem (B.A. Mason and S. Das Sarma), APS March Meeting at Baltimore (1985).
5. An Improved Description of the Physisorption Interaction (S.M. Paik and S. Das Sarma), APS March Meeting at Baltimore (1985).
6. Role of Impurity in the Fractional Quantum Hall Effect: An Exact Numerical Study (F.C. Zhang, V. Vulovic, Y. Guo and S. Das Sarma), APS March Meeting at Baltimore (1985).
7. Hot Electron Phenomena in Semiconductor Microstructures (S. Das Sarma and B.A. Mason), submitted to the 3rd International Conference on Hot electron Effects in Semiconductors (Innsbruck, Austria, July 1985).

II. Proposed Research - Year 2

We plan to work most extensively in the following three areas: (1) Molecular Dynamics simulation of kinetic processes at superlattice interfaces; (2) Epitaxial crystal growth problem; (3) Monte Carlo simulation with particular emphasis on laser-assisted MBE growth. We have all the three projects in various stages of development with preliminary results already available for (1) and (2). We are in the process of developing the computer program for (3). When all the three projects start producing results (in the next three to six months) we can legitimately claim our group to be a leader in the new field of non-equilibrium processes in semiconductor superlattices. We will also pursue our theoretical work on the electronic properties of semiconductor superlattices (with somewhat lower priority since we are already accepted as a leader in this area) by studying some aspects of electronic structure *of* II-VI *and* IV-VI superlattices (in conjunction with experimental projects being funded by the ONR) and by continuing to study the nature of electron-phonon interaction in real structures.

In the next year and a half of this contract, we envision rapid progress (limited only by the available computing facility) in our simulation work involving both the MD and MC analysis. In particular, we are hopeful that our work will provide, for the first time, a global qualitative picture of the dependence of interface kinetics (in the growth of superlattice systems) on various growth parameters (like temperature flux rate, layer number, etc.).

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